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ABSTRACT

The present paper shows how to modify the Kreiss-Oliger 2-4 two-dimensional Leap-Frog scheme so that the allowable time step may be doubled, while the computational complexity remains about the same.

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1. Introduction

In a previous communication [1] (see also [2]), it was shown how the standard multi-dimensional leap-frog finite difference method for solving linear and quasi-linear systems of partial differential equations can be modified so that the stability condition is substantially improved. In particular, it was shown that in the two-dimensional case one can double the time step. The required change in the algorithm is simple to implement, and the resulting modified leap-frog (MLF) algorithm remains convenient to program and requires no more flux vector evaluations than the original leap-frog scheme.

Recently the question arose whether a similar improvement can be achieved for the Kreiss-Oliger 2-4 scheme [3], which is second order accurate in time and has a fourth order spatial accuracy. This scheme is widely used in meteorology and global circulation studies. Its explicitness imposes, of course, a priori restrictions on the time steps and attempts have been made [4] to improve running times by resorting to implicit 2-4 methods [5]. Improvements of a factor of 2 in machine time have been reported, [4]. In this paper we show how a similar improvement may be obtained by modifying the explicit 2-4 scheme in a manner analogous to that reported in [1].

Here we are considering the hyperbolic system

$$\frac{\partial u}{\partial t} = \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = A\frac{\partial u}{\partial x} + B\frac{\partial u}{\partial y}\ , \tag{1}$$

where u, $F(u)$, and $G(u)$ are m component vectors and where A and B are the Jacobians of F and G with respect to u.

The 2-4 Kreiss-Oliger finite difference scheme is the following:

$$u^{n+1}_{j,k} = u^{n-1}_{j,k} + \left(\frac{\Delta t}{\Delta x}\right)\left(-\frac{1}{6}F^n_{j+2,k} + \frac{4}{3}F^n_{j+1,k} - \frac{4}{3}F^n_{j-1,k} + \frac{1}{6}F^n_{j-2,k}\right)$$

$$+ \left(\frac{\Delta t}{\Delta y}\right)\left(-\frac{1}{6}G^n_{j,k+2} + \frac{4}{3}G^n_{j,k+1} - \frac{4}{3}G^n_{j,k-1} + \frac{1}{6}G^n_{j,k-2}\right)$$

$$= u^{n-1}_{j,k} + \left(\frac{\Delta t}{\Delta x}\right)\left[(F^n_{j+1,k} - F^n_{j-1,k}) - \frac{1}{6}(F^n_{j+2,k} - 2F^n_{j+1,k} + 2F_{j-1,k} - F^n_{j-2,k})\right]$$

$$+ \left(\frac{\Delta t}{\Delta y}\right)\left[(G^n_{j,k+1} - G^n_{j,k-1}) - \frac{1}{6}(G^n_{j,k+2} - 2G^n_{j,k+1} + 2G^n_{j,k-1} - G^n_{j,k-2})\right] .$$

$$(1.2)$$

The second term in each of the square brackets serves as a "correction" term to the regular 2-2 leap-frog method and modifies it into a 2-4 scheme, i.e. second order accurate in time and fourth order accurate spatially. The initial value (linear) stability condition for algorithm (1.2) is:

$$\Delta t < \frac{1}{[(\rho(A)/\Delta x) + (\rho(B(/\Delta y))]D} , \qquad (1.3)$$

where $\rho(A)$ and $\rho(B)$ are, respectively, the spectral radii of the coefficient matrices $A = A(u) = \partial F/\partial u$, $B = B(u) = \partial G/\partial u$, which are assumed to be simultaneously symmetrizable. The factor D equals 1.372 ($=f((3/8)^{1/4})$, see (2.6).).

We now seek to modify (1.2) in order to improve (1.3). The best we can hope for is to achieve the one-dimensional stability conditions, namely

$$\frac{\Delta t}{\Delta x} < \frac{1}{\rho(A)D} \quad \text{and} \quad \frac{\Delta t}{\Delta y} < \frac{1}{\rho(B)D} \;. \tag{1.4}$$

2. The Modified Scheme and its Stability

If we introduce the differencing and averaging operators, respectively,

$$\delta_x q_{j,k} = q_{j+\frac{1}{2},k} - q_{j-\frac{1}{2},k}; \qquad \delta_y q_{j,k} = q_{j,k+\frac{1}{2}} - q_{j,k-\frac{1}{2}};$$

$$\mu_x q_{j,k} = (\tfrac{1}{2})(q_{j+\frac{1}{2},k} + q_{j-\frac{1}{2},k}); \quad \mu_y q_{j,k} = (\tfrac{1}{2})(q_{j,k+\frac{1}{2}} + q_{j,k-\frac{1}{2}}),$$

then the scheme (1.2) takes the form

$$u^{n+1}_{j,k} = u^{n-1}_{j,k} + 2(\Delta t/\Delta x)\delta_x\mu_x(1-\tfrac{1}{6}\delta_x^2)F^n_{j,k} + 2(\Delta t/\Delta y)\delta_y\mu_y(1-\tfrac{1}{6}\delta_y^2)G^n_{j,k}. \tag{2.1}$$

Next we review briefly how one establishes the stability limits of (2.1); this will facilitate the treatment of the modified algorithm to be introduced later. If we define a new vector

$$w^n_{j,k} = \begin{pmatrix} u^n_{j,k} \\ v^n_{j,k} \end{pmatrix} \;, \tag{2.2}$$

then the linearized version of the two level finite difference equations (2.1) becomes the following single level system

$$u_{j,k}^{n+1} = v_{j,k}^{n} + 2\lambda_x\mu_x\delta_x(I - \tfrac{1}{6}\delta_x^2)u_{j,k}^{n} + 2\lambda_y\mu_y\delta_y(I - \tfrac{1}{6}\delta_y^2)u_{j,k}^{n},$$
$$v_{j,k}^{n+1} = u_{j,k}^{n}, \tag{2.3}$$

or, equivalently,

$$w_{j,k}^{n+1} = \begin{bmatrix} u_{j,k}^{n+1} \\ v_{j,k}^{n+1} \end{bmatrix} = \begin{bmatrix} 2\lambda_x\mu_x\delta_x(I-\tfrac{1}{6}\delta_x^2) + 2\lambda_y\mu_y\delta_y(I-\tfrac{1}{6}\delta_y^2) & I \\ I & 0 \end{bmatrix} \begin{bmatrix} u_{j,k}^{n} \\ v_{j,k}^{n} \end{bmatrix}, \tag{2.4}$$

where $\lambda_x = A\Delta t/\Delta x$, $\lambda_y = B\Delta t/\Delta y$. Fourier transforming (2.4) we get the following amplification matrix

$$M = \begin{bmatrix} 2i(\lambda_x f(\alpha)+\lambda_y f(\beta)) & I \\ I & 0 \end{bmatrix}, \tag{2.5}$$

where

$$f(z) = 2z\sqrt{1-z^2}\,(1+\tfrac{2}{3}z^2), \quad -1 \leq z \leq 1, \tag{2.6}$$

and $\alpha = \sin(\xi/2)$, $\beta = \sin(\eta/2)$; ξ and η being the dual Fourier variables of the space coordinates x and y.

It may be shown that the stability requirement for M is equivalent to demanding that

$$\rho(\underline{C}) < 1, \tag{2.7}$$

$\rho(\underline{C})$ being the spectral radius of $\underline{C} = A(\Delta t/\Delta x)f(\alpha) +$ $B(\ t/\ y)f(\ )$. We then get

$$\Delta t < \frac{1}{[(\rho(A)/\Delta x) + (\rho(B)/\Delta y)]D}, \tag{2.8}$$

where $D = \max|f(z)| = f(3/8)^{\frac{1}{4}}) = 1.372.$ (2.9)

The most general modification of (2.1) which maintains the fourth order spatial accuracy and still leaves the algorithm with a compact 5x5 grid support $(j\pm 2,\ k\pm 2)$ is:

$$u_{j,k}^{n+1} = u_{j,k}^{n-1} + 2(\Delta t/\Delta x)\mu_x\delta_x(1 - \tfrac{1}{6}\delta_x^2 - \tfrac{\gamma}{16}\delta_x^2\delta_y^2 - \tfrac{\varepsilon}{16}\delta_y^4 - \tfrac{\nu}{64}\delta_x^2\delta_y^4)F_{j,k}^n$$

$$+ 2(\Delta t/\Delta y)\mu_y\delta_y(1 - \tfrac{1}{6}\delta_y^2 - \tfrac{\gamma}{16}\delta_y\delta_x - \tfrac{\varepsilon}{16}\delta_x^4 - \tfrac{\nu}{64}\delta_y\delta_x)G_{j,k}^n \ . \tag{2.10}$$

The amplification matrix again has the form

$$G = \begin{bmatrix} 2i\tilde{C} & I \\ & \\ I & 0 \end{bmatrix} ,$$

where now

$$\tilde{C} = \lambda_x[2\alpha(1-\alpha^2)^{\frac{1}{2}} \cdot (1 + \tfrac{2}{3}\alpha^2 - \gamma\alpha^2\beta^2 - \varepsilon\beta + \nu\alpha^2\beta^4)]$$

$$+ \lambda_y[2\beta(1-\beta^2)^{\frac{1}{2}} \cdot (1 + \tfrac{2}{3}\beta^2 - \gamma\beta^2\alpha^2 - \varepsilon\alpha^4 + \nu\beta^2\alpha^4)].$$

The stability requirement becomes

$$2\rho(\lambda_x)|\alpha|\cdot|1-\alpha^2|^{\frac{1}{2}}\cdot|1+\tfrac{2}{3}\alpha^2-\gamma\alpha^2\beta^2-\varepsilon\beta^4+\nu\alpha^2\beta^4)|$$

$$+\ 2\rho(\lambda_y)|\beta|\cdot|1-\beta^2|^{\frac{1}{2}}\cdot|1+\tfrac{2}{3}\beta^2-\gamma\beta^2\alpha^2-\varepsilon\alpha^4+\nu\beta^2\alpha^4| \leq 1. \quad (2.11)$$

For optimal stability it is required that in contradistinction to (2.8), $\rho(\lambda_x) \leq 1/D$ and $\rho(\lambda_y) \leq 1/D$. We ask whether under these constraints there indeed exists a triplet (γ,ε,ν) such that inequality (2.11) is still valid $\forall\ |\alpha|,|\beta| < 1$. It can be shown that if any member of the triplet (γ,ε,ν) vanishes one cannot get the stipulated optimal stability, (1.4). We found no analytical way to determine a stabilizing triplet. However, we verified numerically that the convenient triplet

$$\gamma = 8,\ \varepsilon = 8/3,\ \nu = 32/3,$$

is appropriate in that it leaves the inequality (2.11) valid under the stipulated optimal stability conditions, eq. (1.4).

Thus, the modified Kreiss-Oliger 2-4 leap-frog scheme takes the form

$$u^{n+1}_{j,k} = u^{n-1}_{j,k} + 2(\Delta t/\Delta x)\delta_x\mu_x(1-\tfrac{1}{6}\delta_x^2-\tfrac{1}{2}\delta_x^2\delta_y^2-\tfrac{1}{6}\delta_y^4-\tfrac{1}{6}\delta_x^2\delta_y^4)F^n_{j,k}$$

$$+\ 2(\Delta t/\Delta y)\delta_y\mu_y(1-\tfrac{1}{6}\delta_y^2-\tfrac{1}{2}\delta_y^2\delta_x^2-\tfrac{1}{6}\delta_x^4-\tfrac{1}{6}\delta_y^2\delta_x^4)G^n_{j,k}. \quad (2.12)$$

Writing out explicitly the effect of the differencing and averaging operators $\delta_x\ \delta_y, \mu_x, \mu_y$, equation (2.12) becomes:

$$
\begin{aligned}
u_{j,k}^{n+1} = u_{j,k}^{n-1} + \frac{1}{6}\left(\frac{\Delta t}{\Delta x}\right)\Big[& -F_{j+2,k+2}^{n}+F_{j+2,k+1}^{n}-F_{j+2,k}^{n}+F_{j+2,k-1}^{n}-F_{j+2,k-2}^{n} \\
& + F_{j+1,k+2}^{n}+2F_{j+1,k+1}^{n}+2F_{j+1,k}^{n}+2F_{j+1,k-1}^{n}+F_{j+1,k-2}^{n} \\
& - F_{j-1,k+2}^{n}-2F_{j-1,k+1}^{n}-2F_{j-1,k}^{n}-2F_{j-1,k-1}^{n}-F_{j-1,k-2}^{n} \\
& + F_{j-2,k+2}^{n}-F_{j-2,k+1}^{n}+F_{j-2,k}^{n}-F_{j-2,k-1}^{n}+F_{j-2,k-2}^{n}\Big] \\
+ \frac{1}{6}\left(\frac{\Delta t}{\Delta y}\right)\Big[& -G_{j+2,k+2}^{n}+G_{j+1,k+2}^{n}-G_{j,k+2}^{n}+G_{j-1,k+2}^{n}-G_{j-2,k+2}^{n} \\
& + G_{j+2,k+1}^{n}+2G_{j+1,k+1}^{n}+2G_{j,k+1}^{n}+2G_{j-1,k+1}^{n}+G_{j-2,k+1}^{n} \\
& - G_{j+2,k-1}^{n}-2G_{j+1,k-1}^{n}-2G_{j,k-1}^{n}-2G_{j-1,k-1}^{n}-G_{j-2,k-1}^{n} \\
& + G_{j+2,k-2}^{n}-G_{j+1,k-2}^{n}+G_{j,k-2}^{n}-G_{j-1,k-2}^{n}+G_{j-2,k-2}^{n}\Big]. \quad (2.13)
\end{aligned}
$$

If we want to emphasize the "modifying" terms which were added to the regular 2-4 scheme we may rewrite (2.13) as follows:

$$\begin{aligned}
u^{n+1}_{j,k} = u^{n-1}_{j,k} &+ \left(\frac{\Delta t}{\Delta x}\right)\Big\{F^n_{j+1,k} - F^n_{j-1,k} - \frac{1}{6}\left[F^n_{j+2,k} - 2F^n_{j+1,k} + 2F^n_{j-1,k} - F^n_{j-2,k}\right] \\
&\quad + \frac{1}{6}\Big[-F^n_{j+2,k+2} + F^n_{j+1,k+2} - F^n_{j-1,k+2} + F^n_{j-2,k+2} \\
&\quad + F^n_{j+2,k+1} + 2F^n_{j+1,k+1} - 2F^n_{j-1,k+1} - F^n_{j-2,k+1} \\
&\quad - 6F^n_{j+1,k} + 6F^n_{j-1,k} \\
&\quad + F^n_{j+2,k-1} + 2F^n_{j+1,k-1} - 2F^n_{j-1,k-1} - F^n_{j-2,k-1} \\
&\quad - F^n_{j+2,k-2} + F^n_{j+1,k-2} - F^n_{j-1,k-2} + F^n_{j-2,k-2}\Big]\Big\} \\
&+ \left(\frac{\Delta t}{\Delta y}\right)\Big\{G^n_{j,k+1} - G^n_{j,k-1} - \frac{1}{6}\left[G^n_{j,k+2} - 2G^n_{j,k+1} + 2G^n_{j,k-1} - G^n_{j,k-2}\right] \\
&\quad + \frac{1}{6}\Big[-G^n_{j+2,k+2} + G_{j+1,k+2} + G^n_{j-1,k+2} - G^n_{j-2,k+2} \\
&\quad + G^n_{j+2,k+1} + 2G^n_{j+1,k+1} - 6G^n_{j,k+1} + 2G^n_{j-1,k+1} + G^n_{j-2,k+1} \\
&\quad - G^n_{j+2,k-1} - 2G^n_{j+1,k-1} + 6G^n_{j,k-1} - 2G^n_{j-1,k-1} - G^n_{j-2,k-1} \\
&\quad + G^n_{j+2,k-2} - G^n_{j+1,k-2} - G^n_{j-1,k-2} + G^n_{j-2,k-2}\Big]\Big\}
\end{aligned} \tag{2.14}$$

Note that even though (2.13) and (2.14) look much more complex than (1.2) one still realizes the benefit of the increased stable time step. This is true when the flux vectors evaluation is costly in terms of machine time, because all the additional fluxes have already been computed at the neighboring points. This can be best seen by defining the following vectors

$$u^{*n}_{j,k} = (1-\frac{3}{8}\delta_x^2\delta_y^2-\frac{1}{8}\delta_y^4-\frac{1}{8}\delta_x^2\delta_y^4)u^n_{j,k}$$
$$u^{**n}_{j,k} = (1-\frac{3}{8}\delta_y^2\delta_x^2-\frac{1}{8}\delta_x^4-\frac{1}{8}\delta_y^2\delta_x^4)u^n_{j,k} \qquad (2.15)$$

In terms of u^* and u^{**} we can construct a different version of the modified 2-4 scheme so that it takes the same form as the standard one (1.2), namely

$$u^{n+1}_{j,k} = u^{n-1}_{j,k}+\left(\frac{\Delta t}{\Delta x}\right)\left[-\frac{1}{6}F^n_{j+2,k}+\frac{4}{3}F^{*n}_{j+1,k}-\frac{4}{3}F^{*n}_{j-1,k}+\frac{1}{6}F^n_{j-2,k}\right]$$
$$+\left(\frac{\Delta t}{\Delta y}\right)\left[-\frac{1}{6}G^n_{j,k+2}+\frac{4}{3}G^{**n}_{j,k+1}-\frac{4}{3}G^{**n}_{j,k-1}+\frac{1}{6}G^n_{j,k-2}\right] \qquad (2.16)$$

where $F^{*n}_{j,k} = F(u^{*n}_{j,k})$, $F^{**n}_{j,k} = F(u^{**n}_{j,k})$ and similarly $G^{*n}_{j,k} = G(u^{*n}_{j,k})$, $G^{**n}_{j,k} = G(u^{**n}_{j,k})$. From (2.15) one can show that (2.16) is equivalent to (2.13) (or (2.14)) to fourth order in space in the nonlinear case. The stability of (2.16) is the same as that of (2.14) since for linear problems they are identical. Notice that the number of flux evaluation is now the same for the modified and the standard 2-4 schemes. The dependent vectors $u^{*n}_{j,k}$ and $u^{**n}_{j,k}$ are evaluated in terms of the neighboring points using only additions of u^n. In particular:

$$u^{*n}_{j,k} = \frac{1}{4}u^n_{j,k} + \frac{1}{8}\Big[-u^n_{j+1,k+2}+u^n_{j,k+2}-u^n_{j-1,k+2}$$

$$+u^n_{j+1,k+1}+2u^n_{j,k+1}+u^n_{j-1,k+1}$$

$$+u^n_{j+1,k-1}+2u^n_{j,k-1}+u^n_{j-1,k-1}$$

$$-u^n_{j+1,k-2}+u^n_{j,k-2}-u^n_{j-1,k-2}\Big] \qquad (2.17)$$

and

$$u^{**n}_{j,k} = \frac{1}{4}u^n_{j,k} + \frac{1}{8}\Big[-u^n_{j+2,k+1}+u^n_{j+1,k+1}+u^n_{j-1,k+1}-u^n_{j-2,k+1}$$

$$+u^n_{j+2,k}+2u^n_{j+1,k}+2u^n_{j-1,k}+u^n_{j-2,k}$$

$$-u^n_{j+2,k-1}+u^n_{j+1,k-1}+u^n_{j-1,k-1}-u^n_{j-2,k-1}\Big] \qquad (2.18)$$

Notice that from a computational point of view, (2.17) and (2.18) can be carried out by observing that certain neighboring points keep appearing together and therefore can be lumped together to reduce the number of additions hence making for a more efficient programming.

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